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ORIGINAL ARTICLE

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A lower bound for a variational model for pattern formation in shape-memory alloys

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Abstract The Kohn-Müller model for the formation of domain patterns in martensitic shape-memory alloys consists in minimizing the sum of elastic, surface and boundary energy in a simplified scalar setting, with a nonconvex constraint representing the presence of different variants. Precisely, one minimizes

$$J_{\varepsilon,\beta}(u) = \beta \|u_0\|^2_{H^{1/2}((0,h))} + \int_{(0,l)\times(0,h)} |\partial_x u|^2 + \varepsilon |\partial_y \partial_y u|$$

among all $u : (0,l) \times (0,h) \to \mathbb{R}$ such that $\partial_y u = \pm 1$ almost everywhere. We prove that for small ε the minimum of $J_{\varepsilon,\beta}$ scales as the smaller of $\varepsilon^{1/2}\beta^{1/2}l^{1/2}h$ and $\varepsilon^{2/3}l^{1/3}h$, as was conjectured by Kohn and Müller. Together with their upper bound, this shows rigorously that a transition is present between a laminar regime at $\varepsilon/l \gg \beta^3$ and a branching regime at $\varepsilon/l \ll \beta^3$.

Keywords Solid-solid phase transformations · Pattern formation · Nonlinear elasticity · Calculus of variations

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1 Introduction

Fine structures arise in many problems in material sciences where a nonconvex bulk energy density with multiple minima is accompanied by boundary conditions, or forcing terms, which favor a convex combination of the minima. In the theory of elasticity and magnetism, this typically results in lamellar patterns (Fig. 1), which can refine close to the boundary (Fig. 2). Such a refinement of the oscillatory pattern toward the boundary was first proposed by Landau back in 1938, in work on the intermediate state of type-I superconductors [1, 2]. Similar patterns were discussed for magnetic domains by Lifshitz in 1944 [3], and later by Hubert [4]. The first mathematical results in this direction have been obtained by Kohn and Müller in 1992–1994 [5, 6] for the case of shape-memory alloys. Their work originated a large amount of mathematical investigations of related pattern-formation problems in materials; for example, similar domain branching has been demonstrated in models of uniaxial ferromagnets [7, 8], thin-film blistering [9–12], diblock copolymers [13, 14], flux domain structures in the intermediate state

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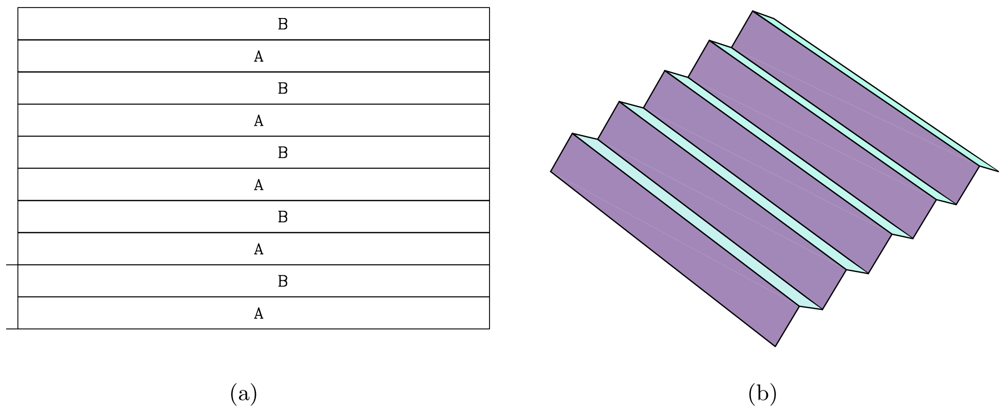

Fig. 1 Sketch of the laminar pattern in for shape-memory alloys. **a** Subdivision of the two-dimensional domain. **b** Three-dimensional representation of the deformation

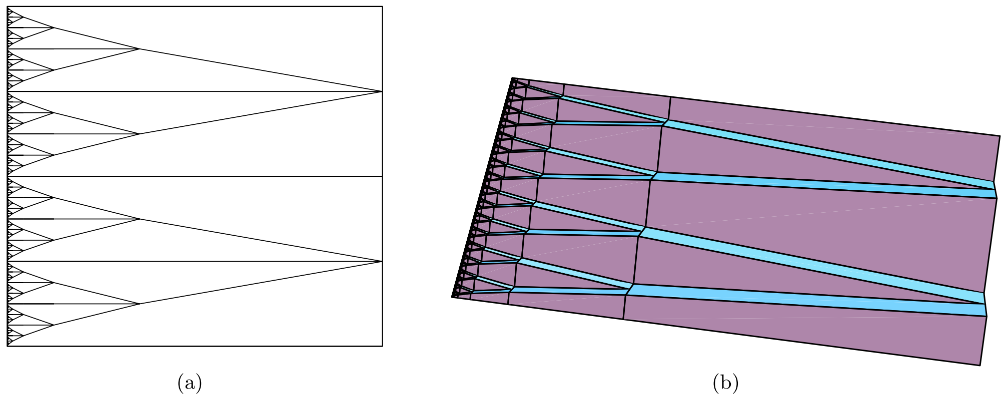

Fig. 2 Branching construction for the model of domains in shape-memory alloys. **a** Subdivision of the domain into the different pieces where u is affine. **b** Three-dimensional representation of the deformation

of type-I superconductor plates [15], and dislocation walls in crystal plasticity [16]. Asymptotic self-similarity of the minima was proven for a simplified version of the Kohn-Müller model, in [17]. Experimental tests were performed in [18]; the results were however, due to high scatter of the data and to the restricted range in which the parameters could be varied, compatible with both the $1/2$ and the $2/3$ scaling laws.

Shape-memory alloys are materials undergoing a solid-solid martensitic phase transition from a high-symmetry phase at high temperature to a low-symmetry one at low temperature [19–21]. The transformation is diffusionless and preserves the crystal structure; in the framework of nonlinear elasticity, each material point can choose between a finite number of the low-symmetry variants, which correspond to different spontaneous strains. If macroscopic deformation is penalized, for example by boundary conditions or by interfaces to other grains in polycrystals, a fine mixture of the different phases is expected. The microstructures typically observed have, at least locally, a laminar structure, as illustrated in Fig. 1. This can be understood as a consequence of the fact that the gradient of a continuous piecewise smooth function can jump from a value $A \in \mathbb{R}^{3\times 3}$ to another one $B \neq A$ across a regular interface only if the jump is of rank one, i.e., if $A - B = a \otimes n$, where n is the normal to the interface. Therefore, the direction of the interface n is determined by the spontaneous strains A and B.

This simple argument shows that some directions are preferred for the interfaces, but does not give any insight into the length scale of the microstructure, or the specific pattern. A more precise picture is obtained including a singular perturbation, corresponding to the energy of domain boundaries, and a term penalizing strong deviations from affine boundary values, representing the elastic energy of the neighboring material. Consider for example, in the domain $(0,1)^2$, the laminar pattern illustrated in Fig. 1, which contains N interfaces along the preferred direction. The energy of the interfaces is given by their length, i.e., N, multiplied by a surface energy density ε. The oscillations on the boundary are penalized by a term measuring the distance of the deformation from affine boundary data, which (in any L^p norm) scales as $1/N$. One obtains

$$E \sim \varepsilon N + \beta \frac{1}{N},$$

where β is a material parameter representing an elastic modulus (a more precise discussion of the second term is given below). Minimization in N gives $N \sim (\beta/\varepsilon)^{1/2}$ and $E \sim (\varepsilon\beta)^{1/2}$. This simple construction scheme, which in the case of magnetic domains goes back to Landau [22], has for many years been the basis of the theoretical understanding of microstructure in shape-memory alloys [19, 23, 24]. The relevance of the more complex, two-dimensional branched pattern was first pointed out by Kohn and Müller [5, 6], who investigated the issue mathematically within a simple scalar model, see Sect. 2. They could prove that with rigid boundary conditions the branched pattern is always favorable (even more, in this case there is no laminar pattern with finite energy). For the more realistic case of a soft boundary condition, i.e., for the model given in (1) below, they conjectured a transition between the laminar and the branched pattern with varying material parameters, and substantiated the conjecture with a rigorous upper bound and a heuristic lower bound. The present work completes this analysis, by providing the remaining lower bound.

2 Model and main result

In the antiplane-shear, thin-wall model by Kohn and Müller [5, 6] one focusses on a scalar component of the deformation, $u : (0,l) \times (0,h) \to \mathbb{R}$, assumes that u_y is the order parameter, and that the two phases can be identified by $u_y = 1$ and $u_y = -1$, respectively, (we write briefly $u_y = \partial_y u$, and analogously u_x, u_{yy}). For each fixed x, the number of interfaces between the two phases is the number of jumps of u_y, which we write as

$$\int_0^h |u_{yy}| dy.$$

This quantity is equivalent to the BV norm of the function $u_y(x,\cdot) : (0,h) \to \{-1,1\}$, which can be defined by

$$\int_0^h |u_{yy}| dy := \sup \left\{ \int_0^h u_y(x,y)\varphi'(y) dy : \varphi \in C_c^1([0,h],[-1,1]) \right\},$$

see, e.g., [25] for a detailed presentation. Variations of the displacement with x are penalized by a purely elastic term, of the form u_x^2. A boundary term accounts for the energetic cost of elastic deformation of the material located outside the domain $(0,l) \times (0,h)$, which has to match continuously with u on the boundary, and achieve zero deformation at infinity. Physically, this represents either a different material, or different grains in a polycrystal, or regions which have not undergone the phase transformation. For simplicity one focusses on the $x = 0$ boundary, and considers an "outside" deformation $v : (-\infty,0) \times (0,h) \to \mathbb{R}$, with elastic energy

$$E_{\mathrm{el}}(v) := \int_{-\infty}^0 \int_0^h |\nabla v|^2 \, dx dy\,.$$

For any given u, one considers the minimum of $E_{\mathrm{el}}(v)$ among all v such that $u = v$ at $x = 0$ (in the sense of traces). This minimum is, by definition, the squared homogeneous $H^{1/2}$ norm of the trace u_0 of u,

$$\|u_0\|^2_{H^{1/2}((0,h))} = \inf\{E_{\mathrm{el}}(v) : v(0,\cdot) = u_0(\cdot)\}.$$

See the Appendix for more details on the $H^{1/2}$ norm, see [5, 6] for a more detailed motivation of the model.

The Kohn-Müller problem is obtained combining the mentioned terms and reads: For given $\varepsilon, \beta > 0$, minimize

$$J_{\varepsilon,\beta}(u) := \beta \|u_0\|^2_{H^{1/2}((0,h))} + \int_{(0,l)\times(0,h)} u_x^2 + \varepsilon |u_{yy}|\, dxdy \tag{1}$$

among all $u \in W^{1,2}((0,l) \times (0,h), \mathbb{R})$ with $|u_y| = 1$ a.e.. Here $u_0(y) = u(0, y)$ in the sense of traces, ε represents the wall energy, and β the relative strength of the material at $x < 0$ with respect to the one at $x > 0$. Kohn and Müller conjectured that, for small ε, the minimum of $J_{\varepsilon,\beta}$ scales as

$$J_0(\varepsilon, \beta) := \min(\varepsilon^{1/2}\beta^{1/2}l^{1/2}, \varepsilon^{2/3}l^{1/3})\, h,$$

in the sense that

$$cJ_0(\varepsilon, \beta) \le \min J_{\varepsilon,\beta}(u) \le c' J_0(\varepsilon, \beta) \tag{2}$$

for some universal constants $c, c' > 0$. The validity of (2) would imply that a transition is present between the regime $\varepsilon/l \gg \beta^3$, where the one-dimensional laminar construction is optimal, and the regime $\varepsilon/l \ll \beta^3$, where the branched construction is optimal.

Besides existence, the upper bound in (2) was proven in [6]. The first term was obtained via the laminar construction discussed above and illustrated in Fig. 1, the second one via the branched construction illustrated in Fig. 2. However, in [6] the lower bound was only proven for a modified functional $\tilde{J}$, where the squared $H^{1/2}$ norm is replaced by $h^{1/2}$ times the L^2 norm of u_0 (unsquared). The two functionals are equivalent provided that

$$\|u_0\|^2_{H^{1/2}} \sim h^{1/2}\|u_0\|_{L^2}.$$

This corresponds to the interpolation inequality

$$\|u_0\|^2_{H^{1/2}} \le \|u_0\|_{L^2}\, \|u_0'\|_{L^2}$$

being sharp for u_0, since by the side condition $u_y = \pm 1$ a.e. one expects the L^2 norm of u_0' to be $h^{1/2}$ (the mentioned interpolation inequality is derived in (9) below). In [6] heuristic arguments were given in this direction, building upon the fact that the interpolation is sharp for approximately periodic functions. We prove here the lower bound in (2), which implies *a posteriori* the correctness of the heuristic argument by Kohn and Müller for the scaling of the minimal energy. Our proof is in many respects analogous to the one used in [16] for a related problem in plasticity, and was first presented in [26].

Theorem 1 *There is a universal constant $c > 0$ such that for any $\varepsilon, \beta, l, h > 0$ and any $u \in W^{1,2}((0,l) \times (0,h))$ with $u_y = \pm 1$ a.e. one has*

$$J_{\varepsilon,\beta}(u) \ge c \min(\varepsilon^{1/2}\beta^{1/2}l^{1/2}, \varepsilon^{2/3}l^{1/3}, \beta)\, h.$$

3 Proof

The idea of the proof is to divide the domain into horizontal stripes $(0, l) \times (y, y + \lambda)$, whose width λ is given by the maximal width of a layer in the domain. In each stripe, at least one of the following holds: either (i) there is at least one long interface (thereby making the singular perturbation large), or (ii) the elastic energy is large, or (iii) the trace is approximately affine with slope one, rendering the boundary term large. Balancing these three terms will give the desired lower bound. Here and below c and c' denote universal constants, which might change from line to line.

Point (iii) will be treated via the following lemma.

Lemma 1 *There is a universal constant $c > 0$ such that for any $\lambda > 0$, any $u : (0, \lambda) \to \mathbb{R}$, and any constant $\bar{u} \in \mathbb{R}$, one has*

$$\|u(y) - y - \bar{u}\|_{L^1((0,\lambda))} + \|u(y)\|^2_{H^{1/2}((0,\lambda))} \ge c\lambda^2.$$

Proof By scaling $\tilde{u}(y) = \lambda u(y/\lambda)$ it is sufficient to prove the statement for $\lambda = 1$, and adding a constant to u and $\bar{u}$ we can assume that $\int_0^\lambda u\,dy = 0$. We proceed by contradiction. If the thesis were false, there would be sequences $u_j \in L^1$, $\bar{u}_j \in \mathbb{R}$ such that $u_j - \bar{u}_j \to y$ in $L^1((0,1))$, and $u_j \to 0$ in $H^{1/2}((0,1))$. The latter implies $u_j \to 0$ in $L^1((0,1))$, a contradiction.

Proof (of Theorem 1) By scaling $\tilde{u}(x, y) = hu(x/h, y/h)$, $\tilde{\varepsilon} = \varepsilon/h$, $\tilde{l} = l/h$, it suffices to prove the result for the case $h = 1$. We fix some $\lambda \in (0,1)$, and choose an interval $\mathcal{I} = (y, y+\lambda) \subset (0,1)$ so that the slice energy satisfies

$$E_{\mathcal{I}} := \beta\|u_0\|^2_{H^{1/2}(\mathcal{I})} + \int_{(0,l)\times\mathcal{I}} u_x^2 + \varepsilon|u_{yy}| \le 2\lambda E$$

where $E = J_{\varepsilon,\beta}(u)$ is the total energy. This is always possible since the squared $H^{1/2}$ norm is super-additive, see (8) below. We next exploit the fact that for a fixed x, the number of jumps of the function $u_y(x,\cdot)$ must be an integer. Precisely, for a.e. $x \in (0,l)$, the function $u_y(x,\cdot)$ is a function of bounded variation which takes values ± 1, hence

$$\int_{\{x\}\times\mathcal{I}} |u_{yy}| \in \mathbb{N} \text{ for a.e. } x, \tag{3}$$

see e.g., [25]. If the integral in (3) is nonzero for almost every $x \in (0,l)$, then

$$E_{\mathcal{I}} \ge l\varepsilon. \tag{4}$$

Otherwise, there is a set of positive measure $\mathcal{N} \subset (0,l)$ such that either

$$u(x, y) = \bar{u}(x) + y \qquad \text{on } \mathcal{N}\times\mathcal{I} \tag{5}$$

or $u(x,y) = \bar{u}(x) - y$ on $\mathcal{N}\times\mathcal{I}$, for some $\bar{u} : \mathcal{N} \to \mathbb{R}$. In the following, we assume for definiteness that the first option holds (the other case is clearly equivalent). For a.e. $x \in (0,l)$ we have

$$\begin{aligned}\|u_0(\cdot) - u(x,\cdot)\|_{L^1(\mathcal{I})} &\le \|\partial_x u\|_{L^1((0,l)\times\mathcal{I})}\\ &\le (l\lambda)^{1/2}\|\partial_x u\|_{L^2((0,l)\times\mathcal{I})} \le (E_{\mathcal{I}} l\lambda)^{1/2}.\end{aligned}$$

Combining with (5) we obtain

$$\|u_0(y) - y - \bar{u}\|_{L^1(\mathcal{I})} \le (E_{\mathcal{I}} l\lambda)^{1/2},$$

for some $\bar{u} \in \mathbb{R}$. Lemma 1 implies

$$\|u_0(y) - y - \bar{u}\|_{L^1(\mathcal{I})} + \|u_0(y)\|^2_{H^{1/2}(\mathcal{I})} \ge c\lambda^2,$$

which gives

$$(E_{\mathcal{I}} l\lambda)^{1/2} + \frac{E_{\mathcal{I}}}{\beta} \ge c\lambda^2. \tag{6}$$

Combining (4) and (6), and using that $E \ge E_{\mathcal{I}}/(2\lambda)$, we get that for any $\lambda \in (0,1)$

$$E \ge c\min\left(\frac{l\varepsilon}{\lambda}, \beta\lambda, \frac{\lambda^2}{l}\right).$$

If ε is small, in the sense that

$$\varepsilon \le \min\left(\frac{\beta}{l}, \frac{1}{l^2}\right),$$

we can choose

$$\lambda = \max\left(\left(\frac{l\varepsilon}{\beta}\right)^{1/2}, l^{2/3}\varepsilon^{1/3}\right)$$

and obtain

$$E \geq c \min((l\varepsilon\beta)^{1/2}, l^{1/3}\varepsilon^{2/3}).$$

Otherwise, we choose $\lambda = 1$, and get

$$E \geq c \min\left(l\varepsilon, \beta, \frac{1}{l}\right).$$

In this minimization, only the middle term is relevant. Indeed, the first one is – for these values of ε – always larger than one of the other two. Further, the energy is an increasing function of l. In particular, if some u is admissible for a value of $l > 1/\beta$, then its restriction is admissible for $l' = 1/\beta$, and its energy is no larger. Therefore we can put $l = 1/\beta$ in the above estimate (this corresponds to using only the values of $x \in (0, 1/\beta)$ in (3) and the following discussion). We conclude

$$E \geq c \min((l\varepsilon\beta)^{1/2}, l^{1/3}\varepsilon^{2/3}, \beta).$$

The constructions showing optimality of the first and second term have been discussed above and are illustrated in Figs. 1 and 2, and correspond, respectively, to a laminar and to a branched microstructure. The third term is optimal in the regime of very small β, where the material decouples from the boundary condition, and corresponds to a trivial affine deformation, such as $u(x, y) = y$.

Appendix A: Some properties of the $H^{1/2}$ norm

We recall below the definition and the basic properties of the $H^{1/2}$ norm, following the lines of the Appendix to [6].

The homogeneous $H^{1/2}$ norm of a function $u : (a, b) \to \mathbb{R}$ is defined as the infimum of the elastic energy $E_{\mathrm{el}}(v)$ defined in the Introduction among all $v : (-\infty, 0) \times (a, b) \to \mathbb{R}$ such that $u = v$ at $x = 0$ (in the sense of traces). Precisely,

$$\|u\|^2_{H^{1/2}((a,b))} := \inf\left\{\int_{-\infty}^0 \int_a^b |\nabla v|^2\, dx dy \ :\ \ v(0, y) = u(y)\right\}. \tag{7}$$

This norm is subadditive, in the sense that for all $c \in (a, b)$ we have

$$\|u\|^2_{H^{1/2}((a,c))} + \|u\|^2_{H^{1/2}((c,b))} \leq \|u\|^2_{H^{1/2}((a,b))}. \tag{8}$$

To see this, consider any function $v : (-\infty, 0) \times (a, b) \to \mathbb{R}$ entering the infimum in the definition (7), for $\|u\|^2_{H^{1/2}((a,b))}$. Then, the restriction of v to $(-\infty, 0) \times (a, c) \to \mathbb{R}$ is one of the test functions entering the definition of $\|u\|^2_{H^{1/2}((a,c))}$, and analogously on the other interval. Since

$$\int_{-\infty}^0 \int_a^c |\nabla v|^2\, dx dy + \int_{-\infty}^0 \int_c^b |\nabla v|^2\, dx dy = \int_{-\infty}^0 \int_a^b |\nabla v|^2\, dx dy\,,$$

the claimed (8) follows.

The minimization entering (7) can be performed explicitly using Fourier series. In order to have a simple, classical treatment in the case that u is smooth, we first embed it in a periodic setting; for notational simplicity we do this only on the interval $(0, h)$. Then it suffices to extend u to an even, $2h$-periodic function. Precisely, we set $u(-y) = u(y)$ for $y \in [0, h]$, and $u(y + 2h\mathbb{Z}) = u(y)$ for $y \in [-h, h]$. If the original u is continuous, then the extension is continuous and periodic. The same can be done, working at fixed x, to any $v : (-\infty, 0) \times (0, h)$. The condition $v(0, y) = u(y)$ is clearly preserved by the extension.

Let now $v_k(x)$ be the Fourier coefficients of the function $v(x, \cdot)$ on the interval $(-h, h)$, i.e., be such that

$$v(x, y) = \sum_{k\in\mathbb{Z}} e^{i\pi ky/h} v_k(x)\,,$$

and analogously u_k. Since v is real and even in y, we have $v_{-k} = v_k \in \mathbb{R}$. Plancherel's formula gives

$$\frac{1}{2}\int_{-h}^h v^2(x, y)\, dy = h \sum_{k\in\mathbb{Z}} |v_k|^2(x)\,,$$

for any x. Applying this to the gradient of v we obtain

$$E_{\rm el}(v) = \frac{1}{2}\int_{-\infty}^{0}\int_{-h}^{h} |\nabla v|^2\, dxdy = h\int_{-\infty}^{0} \sum_{k\in\mathbb{Z}} \frac{\pi^2 k^2}{h^2}|v_k|^2(x) + |v_k'|^2(x)dx\,.$$

This way the different wavelengths k decouple. The resulting one-dimensional variational problems can be explicitly solved. Incorporating the boundary condition $v_k(0) = u_k$, the minimizer is $\bar v_k(x) = u_k e^{\pi |k| x/h}$. The $H^{1/2}$ norm can therefore be written as

$$\|u\|^2_{H^{1/2}((0,h))} = \inf\{E_{\rm el}(v) : v(0,\cdot) = u(\cdot)\} = \pi\sum_{k\in\mathbb{Z}} |k||u_k|^2\,.$$

Finally, using the Cauchy-Schwartz inequality and Plancherel's formula for the L^2 norms of u and its derivative, we obtain the interpolation inequality

$$\begin{aligned}\pi\sum_{k\in\mathbb{Z}}|k||u_k|^2 &= \pi\sum_{k\in\mathbb{Z}}(|k||u_k|)\cdot|u_k| \\ &\le \left(h\sum_{k\in\mathbb{Z}}|u_k|^2\right)^{1/2}\left(h\sum_{k\in\mathbb{Z}}\frac{\pi^2k^2}{h^2}|u_k|^2\right)^{1/2} = \|u\|_{L^2((0,h))}\,\|u'\|_{L^2((0,h))}\,. \end{aligned} \tag{9}$$

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